Modeling the Vibrational Dynamics and Nonlinear Infrared Spectra of Coupled Amide I and II Modes in Peptides

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Supplementary data for A.G. Dijkstra, T.l.C. Jansen and J. Knoester, "Modeling the vibrational dynamics and nonlinear infrared spectra of coupled amide I and II modes in peptides"

This file contains the data for the nearest neighbor coupling maps, which are shown in Figs. 6 and 7 in the main text.

% Dihedral angles
phis = [0, 30, 60, 90, 120, 150, 180];
psis = [-150, -120, -90, -60, -30, 0, 30, 60, 90, 120, 150, 180];

% Each row of data contains the symmetrized Hamiltonian in cm-1 for a (phi, psi) pair.
% the order of the rows is (phis[0], psis[0]); (phis[0], psis[1]) until (phis[0], psis[max]);
% then (phis[1], psis[0]) et cetera.

% The order of the columns is
% C-site amide II frequency, II-II coupling, C-site I-II coupling, N-site I - C-site II,
% II-II coupling (*), N-site amide II frequency, C-site I - N-site II, N-site I-II coupling,
% C-site I-II coupling (*), C-site I - N-site II (*), C-site am I frequency, I-I coupling,
% N-site I - C-site II (*), N-site I-II coupling (*), I-I coupling (*), N-site am I freq (*).
% Because each line contains a full (symmetric) Hamiltonian, the off-diagonal elements appear twice,
% as indicated with (*).

1340.3, -3.7, -15.4, 2.8, -3.7, 1375.4, -1.5, 2.2, -15.4, -1.5, 1650.9, 13.6, 2.8, 2.2, 13.6, 1640.4
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